

Diethyl ether

60-29-7 | DTXSID3021720

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.85 | 0.69 | 0.86 | 0.67 | 0.86 | 0.78 |

Model Results

Predicted value: 9.83e-01

Global applicability domain: Inside

Local applicability domain index: 6.37e-01

Confidence level: 8.06e-01

Nearest Neighbors from the Training Set

| | | |
|---|--|---|
| <div>Image not found</div> <div>Diethyl ether</div> <div>Measured: 0.89</div> <div>Predicted: 9.83e-01</div> | <div>Image not found</div> <div>Propane, 1-methoxy-</div> <div>Measured: 1.21</div> <div>Predicted: 1.07</div> | <div>Image not found</div> <div>Butane, 1-methoxy-</div> <div>Measured: 1.66</div> <div>Predicted: 1.49</div> |
| <div>Image not found</div> <div>N-Methyl-N-propylamine</div> <div>Measured: 0.84</div> <div>Predicted: 7.94e-01</div> | <div>Image not found</div> <div>Ethylene glycol diethyl ether</div> <div>Measured: 0.66</div> <div>Predicted: 6.93e-01</div> | |